2. To: (Receiving Organization)	3. From: (Originating Organization)	4. Related EDT No.:
C-106 Retrieval Project	ARES Corporation	N/A

5. Proj./Prog./Dept./Div.:	6. Design Authority/Design Agent/Cog. Engr.:	7. Purchase Order No.:
C-106 Retrieval Project	G. Janicek	N/A

8. Originator Remarks:

241-C-106 Retrieval, Molar Fraction of Oxalic Acid in Vapor Phase.

9. Equip./Component No.: N/A

10. System/Bldg./Facility: 241-C-106

12. Major Assm. Dwg. No.: N/A

11. Receiver Remarks: 11A. Design Baseline Document? ☒ Yes ☐ No

13. Permit/Permit Application No.: N/A

14. Required Response Date: N/A

15. DATA TRANSMITTED

(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	(F) Approval Desig-nator	(G) Reason for Trans-mittal	(H) Origi-nator Dispo-sition	(I) Receiv-er Dispo-sition
1	RPP-16994		O	Molar Fraction of Oxalic Acid in the Vapor Phase for Tank 241-C-106 Acid Dissolution Project	N/A	1	1	

16. KEY

Approval Designator (F)	Reason for Transmittal (G)	Disposition (H) & (I)
E, S, Q, D OR N/A (See WHC-CM-3-5, Sec. 12.7)	1. Approval 4. Review 2. Release 5. Post-Review 3. Information 6. Dist. (Receipt Acknow. Required)	1. Approved 4. Reviewed no/comment 2. Approved w/comment 5. Reviewed w/comment 3. Disapproved w/comment 6. Receipt acknowledged

17. SIGNATURE/DISTRIBUTION
(See Approval Designator for required signatures)

(G) Rea-son	(H) Disp.	(J) Name (K) Signature (L) Date (M) MSIN	(G) Rea-son	(H) Disp.	(J) Name (K) Signature (L) Date (M) MSIN
1	/	Design Authority G. Janicek 8/5/03 S7-12	1	/	J. Bellomy 8/2/03 S7-24 R2-11
1	/	Design Agent M. White for Elliot 7-25-03 ARES	1	/	J. Propson 7/26/03 S7-90
1	/	Cog. Eng. B. Barton WD Barton 7/23/03 S7-90			
1	/	Cog. Mgr. W. Thompson J. Propson John Propson for Thompson per telecon 7/26/03 S7-65	3		R. Gustavson X2-09
		QA			
		Safety			
		Env.			

18.	19.	20.	21. DOE APPROVAL (if required)
M.A. White 7-25-03 Signature of EDT Originator Date	Authorized Representative Date for Receiving Organization	G. Janicek 8/5/03 Design Authority/ Cognizant Manager Date	Ctrl No. _____ ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments

BD-7400-172-2 (10/97)

BD-7400-172-1

Molar Fraction of Oxalic Acid in Vapor Phase for Tank 241-C-106 Acid Dissolution Project

White, M. A.
CH2M Hill Hanford Group, Inc.
Richland, WA 99352
U.S. Department of Energy Contract DE-AC27-99RL14047

EDT/ECN: 636798   UC: N/A
Cost Center: N/A   Charge Code: 501555
B&R Code: N/A   Total Pages: 21

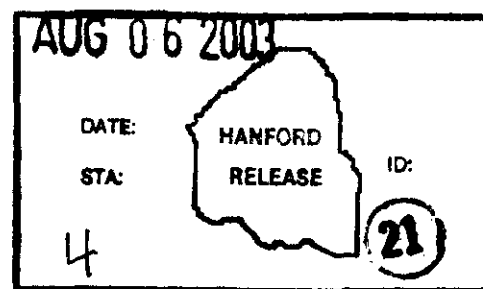Key Words: Oxalic acid, acid dissolution, henry's law, vapor phase, C-106 241-C-106

Abstract: The purpose of this calculation is to calculate the molar fraction of oxalic acid in vapor phase for Tank 241-C-106 acid dissolution project.

AUG 0 6 2003

DATE: HANFORD
STA: RELEASE   ID:
4   (21)

Release Approval   8/6/03   Date   Release Stamp

Approved For Public Release

Subject: C-106 Acid Dissolution Waste Retrieval System

The subject document has been reviewed by the undersigned.
The checker reviewed and verified the following items as applicable.

Documents Reviewed: RPP-16994, Rev. 0 *Molar Fraction of Oxalic Acid in Vapor Phase for Tank 241-C-106 Acid dissolution Project*

Analysis Performed By: Ares Corporation

- Design Input
- Basic Assumptions
- Approach/Design Methodology
- Consistency with item or document supported by the calculation
- Conclusion/Results Interpretation
- _____

Checker (printed name, signature, and date) W. B. Barton *W.B. Barton* 7/31/03

Organizational Manager (printed name, signature and date)

W T Thompson _____ 7/31/03

MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK 241-C-106 ACID DISSOLUTION PROJECT

			SHEET 1 OF 2
A R E S CORPORATION	**CALCULATION COVER SHEET**		CALCULATION NO: 0193101.07-CH-001

PROJECT TITLE/NUMBER: 241-C-106 Acid Dissolution Project 0193101.07	CLIENT: CH2M Hill Hanford Group, Inc.

TITLE:

MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK C-106 ACID DISSOLUTION PROJECT

PURPOSE AND OBJECTIVE:

The purpose of this calculation is to determine the molar fraction of oxalic acid in the vapor phase. This calculation will be used to assist the materials compatibility assessment for equipment that will be exposed to the oxalic acid vapor.

REV. No.	REVISION DESCRIPTION (ADD CONTINUATION SHEET IF REQUIRED)	PREPARED BY NAME/DATE	REVIEWED BY NAME/DATE	PM/TL APPROVAL/DATE
0	Initial Release	M. Feldmann 7/17/03	B. Groth 7/21/03	M. White 7/21/03
1	Clarification of Assumption Minor Editorial Changes	M. Feldmann *Monika Feldmann* 7/22/03	T. Salzano *[signature]* 7/22/03	M. White *[signature]* 7/22/03

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CALCULATION
REVIEW CHECKLIST

CALC NO.: _____0193101.07-CH-001_____ REVISION NO.: ____1____ SHEET NO.: _2_ OF _2_

ITEMS CHECKED	ACCEPT			INITIAL/DATE
	Y	N	N/A	
1. Cover sheets properly completed.	✓			
2. Calc sheet headers complete with calc no, rev, etc.	✓			
3. Calc sheet contents complete per format.	✓			
4. Listed attachments included.	✓			
5. Calc objective clearly described.	✓			
6. Criteria are suitable and properly referenced to task specific documents.	✓			
7. Assumptions and input data described and attached or referenced to task documents.	✓			
8. Calc method identified and appropriate for the design activity.	✓			
9. Calc results reasonable and correctly described in results and conclusions.	✓			
10. Computer program identified with version and revision.	✓			
11. Computer input/output provided or referenced.	✓			
12. Computer run traceable to calculation (file #, etc.).			✓	MathCAD verified by hand calculation
13. Computer input data within permissible design input range.	✓			
14. Computer program validation/verification addressed.			✓	MathCAD verified by hand calculation

DISCREPANCIES / COMMENTS

CHECKER
B. GROTH T. SALZANO _[signature]_
PRINT NAME AND SIGN

_7/22/03_
DATE

ORIGINATOR
M. FELDMANN _Monita Feldmann_
PRINT NAME AND SIGN

_7/22/03_
DATE

Signatures obtained only after discrepancies are corrected and comments are resolved.

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CALCULATION SHEET

Background/Purpose

Oxalic acid ($C_2H_2O_4$) will be introduced into tank 241-C-106. Oxalic acid will be added to the tank in 30,000 gallon increments and allowed to soak. The soak time of the first acid addition is anticipated to be approximately one to two days. Subsequent acid additions will remain in the tank for up to one week. During the soak time, the acid will be gently agitated/re-circulated within the tank.

The purpose of this calculation is to determine the molar fraction of oxalic acid in the vapor phase. This calculation will be used to assist the materials compatibility assessment for equipment that will be exposed to the oxalic acid vapor.

Design Inputs

1. Molarity of Oxalic Acid: 0.91 M
2. Molecular Weight of Oxalic Acid: 90.02 grams/mol
3. Henry's Law constant: 6.908×10^4 mol·m^{-3}/Pa (See Attachment A)
4. Tank Temperature: ~25°C (See Attchment B)
5. Maximum Atmospheric Pressure: 30.23 in Hg (PNNL-14242)
6. Minimum Atmospheric Pressure: 28.15 in Hg (PNNL-14242)
7. Maximum Allowable Vacuum for Tank C-106: 0.8 in water, 0.06 in Hg (OSD-T-151-00013)

Methodology

Henry's law is applicable for real solutions at low concentrations. The law states that the amount of a gas that dissolves in a liquid is proportional to the partial pressure of the gas over the liquid, provided no chemical reaction takes place between the liquid and the gas. Essentially, the gas will diffuse across a gas-fluid interface until the partial pressure is the same on both sides.

$$p_A = y_A P = x_A K_h(T)$$

Where,

p_a = Partial pressure of A in the gas phase
y_A = Mole fraction of A in the gas phase
P = System Pressure
x_A = Mole fraction of A in the liquid phase
$K_h(T)$ = Henry's law constant for A at a specific temperature
T = Temperature

Hand calculations were performed with the assistance of MathCAD software

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CALCULATION SHEET

PROJECT NO.: ACID DISSOLUTION	CALC NO.: 0193101.07-CH-001	REVISION NO.: 1	SHEET NO.: 4 OF 7

SUBJECT: MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK C-106 ACID DISSOLUTION PROJECT

PREPARED BY: M. FELDMANN   DATE: 7/17/03   REVIEWED BY: T.SALZANO   DATE: 7/22/03

Assumptions

This analysis assumes that due to the design of the in-tank chemical mixing assembly and acid addition system, where introduction of acid occurs below the liquid surface level, minimal potential aerosols will be generated from the re-circulation loop during waste retrieval using the acid dissolution process. Additional assumptions are described throughout the calculation.

Results/Conclusions

The result of this calculation showed that the maximum molar fraction of oxalic acid in the vapor phase is 2.239×10^{-9}. The molar fraction was bounded using the maximum and minimum tank pressures accounting for the vacuum induced by the exhauster system.

References

Boyles, V. C., 2003, OSD-T-151-00013, "Operating Specifications for Single-Shelll Waste Storage Tanks." CH2M Hill Hanford Group, Inc., Richland, Washington.

Felder, R.M. and R.W. Rousseau, 1986, "Elementary principles of Chemical Processes, Second Edition." John Wiley & Sons, New York, New York.

Hoitink, D. J., et al., 2003, PNNL-14242, "Hanfor Site Climatological Data Summary 2002 with Historical Data." Pacific Northwest National Laboratory, Richland, Washington.

Perry, R.H. and D.W Green, 1984, "Perry's Chemical Engineers' Handbook, Sixth Edition." McGraw-Hill Book Company, New York, New York.

Sander, R., 1999, "Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry." Air Chemistry Department Max-Planck Institute of Chemistry, Germany. (Attachment A).

Tank Waste Information Network System (TWINS), Queried 06/24/03, [Tank 241-C-106, Temperature Data from 6/10/03 to 6/16/03, Fahrenheit], http://twins.pnl.gov:8001/twins.htm.

CALCULATION SHEET

A R E S
C O R P O R A T I O N

PROJECT NO.: __ACID DISSOLUTION__   CALC NO.: __0193101.07-CH-001__   REVISION NO.: __1__   SHEET NO.: 5 OF 7

SUBJECT: __MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK C-106 ACID DISSOLUTION PROJECT__

PREPARED BY: __M. FELDMANN__   DATE: 7/17/03   REVIEWED BY: __T. SALZANO__   DATE: 7/22/03

Composition of oxalic acid in liquid and vapor phases:

Design Inputs:

$T := 25\,C$ Temperature

$MW_{ox} := 90.02\,\dfrac{gm}{mol}$ Molecular weight of Oxalic Acid

$m_{ox} := 0.91\,\cdot\dfrac{mol}{L}$ m_{ox} = Molarity oxalic acid

$P_{max} := 30.23\,\cdot in\_Hg$ Tank C-106 is vented to the atmosphere. The maximum tank pressure is equal to the maximum atmospheric pressure.

$\quad\quad P_{max} = 765.683\;\;torr$

$P_{vac} := 0.06\,\cdot in\_Hg$ The maximum vacuum allowed for Tank C-106 is 0.8 in water (0.06 in Hg).

$\quad\quad P_{vac} = 1.52\;\;torr$

$P_{min} := 28.15\,\cdot in\_Hg - P_{vac}$ The minimum tank pressure is the minimum atmospheric pressure less the maximum allowable tank vacuum.

$\quad\quad P_{min} = 711.48\;\;torr$

Conversions:

1 in Hg = 25.329 torr
1 torr = 133.322 Pa

Calculation of mass fraction of oxalic acid from molarity:

Basis: 1L Water = 1000gm Water

$mass_{moles} := m_{ox}\cdot\left(MW_{ox}\right)\cdot 1\,L$ $mass_{moles}$ = mass of mole in basis

$\quad\quad mass_{moles} = 81.918\;\;gm$

$massfract_{ox} := \dfrac{mass_{moles}}{1000\;gm + mass_{moles}}$ $massfract_{ox}$ = mass fraction of acid in basis

$\quad\quad massfract_{ox} = 0.076$

PROJECT NO.: __ACID DISSOLUTION__   CALC NO.: __0193101.07-CH-001__   REVISION NO.: __1__   SHEET NO.: 6 OF 7

SUBJECT: __MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK C-106 ACID DISSOLUTION PROJECT__

PREPARED BY: __M. FELDMANN__   DATE: 7/17/03   REVIEWED BY: __T.SALZANO__   DATE: 7/22/03

Conversion of mass fraction to mole fraction of oxalic acid in the liquid phase:

$$n_{ox} := \left(massfract_{ox}\right) \cdot \frac{(1mol)}{90.02\,gm} \cdot 100gm \qquad n_{ox} = \text{moles acid in liquid phase}$$

$$n_{ox} = 0.084 mol$$

$$n_{h2o} := 100gm \cdot \left(1 - massfract_{ox}\right) \frac{(1mol)}{18.01gm} \qquad n_{h2o} = \text{moles of water in liquid phase}$$

$$n_{h2o} = 5.132 mol$$

$$n_t := n_{ox} + n_{h2o} \qquad n_t = \text{total moles for 100 gram of solution (basis)}$$

$$n_t = 5.216 mol$$

$$x_{ox} := \frac{n_{ox}}{n_t}$$

$$x_{ox} = 0.016 \qquad x_{ox} = \text{mole fraction of oxalic acid in liquid phase}$$

$$x_{h2o} := \frac{n_{h2o}}{n_t} \qquad x_{h2o} = \text{mole fraction of water in liquid phase}$$

$$x_{h2o} = 0.984$$

Henry's law is valid for dilute solutions, providing that A does not dissociate, ionize, or react in the liquid phase.

Henry's Law $$p_{ox} = y_{ox}P = x_{ox} K_{H(T)}$$

Where

p_{ox} = partial pressure

P   = system pressure

y_{ox} = mole fraction in vapor phase

x_{ox} = mole fraction in liquid phase

$K_{H(T)}$ = Henry's Law Constant at T

Henry's Law Constant:

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SHEET

PROJECT NO.: __ACID DISSOLUTION__   CALC NO.: __0193101.07-CH-001__   REVISION NO.: __1__   SHEET NO.: 7 OF 7

SUBJECT: __MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK C-106 ACID DISSOLUTION PROJECT__

PREPARED BY: __M. FELDMANN__   DATE: 7/17/03   REVIEWED BY: __T.SALZANO__   DATE: 7/22/03

Henry's Law Constant:

$$K_H := 7.0 \times 10^6 \cdot \frac{M}{atm}$$

K_H, Henry's Law Constant for Oxalic acid in terms of concentration in the aqueous phase and the partial pressure at T=25 C from Table on page A-7 of Attachment A. The bounding value for the constant was used.

Where

$$M = mol/dm^3$$

Conversion of Henry's Law Constant (K_H) to units of torr, K_{Hpx}. Where K_{Hcp} is in terms of aqueous concentration and partial pressure and K_{Hpx} is in terms of partial pressure and the molar fraction of the acid:

$$K_{Hcp} := \frac{K_H}{101.325}$$

Equation 6, page A-4 from Attachment A

$$K_{Hcp} := 6.908 \times 10^4 \cdot \frac{\left(\frac{mol}{m^3}\right)}{Pa}$$

$$K_{Hpx} := \frac{1}{\left[K_{Hcp} \cdot \frac{(1 \cdot L)}{0.91 \cdot mol} \cdot \frac{(1 \cdot m^3)}{1000 \cdot L}\right]}$$

Conversion of Henry's Law Constant to units of Torr

$$K_{Hpx} = 9.881 \times 10^{-5} \, torr$$

The maximum and minimum tank pressures are used to bound and solve for molar fraction of oxalic acid in the vapor phase using Henry's Law.

$$y_{ox1} := \frac{(x_{ox} \cdot K_{Hpx})}{P_{max}}$$

y_{ox1} = mole fraction of oxalic acid in vapor phase using the maximum tank pressure.

$$y_{ox1} = 2.081 \times 10^{-9}$$

$$y_{ox2} := \frac{(x_{ox} \cdot K_{Hpx})}{P_{min}}$$

y_{ox1} = mole fraction of oxalic acid in vapor phase using the minimum tank pressure.

$$y_{ox2} = 2.239 \times 10^{-9}$$

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CALCULATION SHEET

PROJECT NO.: __ACID DISSOLUTION__   CALC NO.: __0193101.07-CH-001__   REVISION NO.: __1__   SHEET NO.: 1 OF 7

SUBJECT: __MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK C-106 ACID DISSOLUTION PROJECT__

PREPARED BY: __M. FELDMANN__   DATE: 7/17/03   REVIEWED BY: __T.SALZANO__   DATE: 7/22/03

Attachment A

Excerpts from "Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry"

Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry

http://www.mpch-mainz.mpg.de/~sander/res/henry.html

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Version 3 (April 8, 1999)

Contents

1   Introduction

Henry's law constants (solubilities) of trace gases of potential importance in environmental chemistry (atmospheric chemistry, waste water treatment, ...) have been collected and converted into a uniform format.

Disclaimer: Although this compilation has been edited with greatest care the possibility of errors cannot be excluded. If you use data from this table it is recommended that you also check the original literature. If you find an error in this table, please tell me about it!

2   The physical quantity of solubility

There are several ways of describing the solubility of a gas in water. Usually the Henry's law constant k_H is defined as:

$$k_H \stackrel{\text{def}}{=} c_a/p_g \tag{1}$$

Here, c_a is the concentration of a species in the aqueous phase and p_g is the partial pressure of that species in the gas phase. If k_H refers to standard conditions ($T^{\ominus} = 298.15$ K) it will be denoted as $k_H^{\ominus}$.

Henry's law constant can also be expressed as the dimensionless ratio between the aqueous-phase concentration c_a of a species and its gas-phase concentration c_g:

$$k_H^{cc} \stackrel{\text{def}}{=} c_a/c_g = k_H \times RT \tag{2}$$

where R = gas constant and T = temperature. To distinguish these different physical quantities, this constant has been named k_H^{cc} here.

Sometimes the reciprocal value $k_{H,inv}^{px}$ is used, representing the volatility instead of the solubility. The usual definition is:

$$k_{H,inv}^{px} \stackrel{\text{def}}{=} p_g/x_a = \frac{\varrho_{H_2O}}{M_{H_2O} \times k_H} \tag{3}$$

where x_a = molar mixing ratio in the aqueous phase, ϱ_{H_2O} = density of water, and M_{H_2O} = molar mass of water.

3   Temperature dependence

A simple way to describe Henry's law as a function of temperature is:

$$k_H = k_H^{\ominus} \times \exp\left(\frac{-\Delta_{soln}H}{R}\left(\frac{1}{T} - \frac{1}{T^{\ominus}}\right)\right) \tag{4}$$

where $\Delta_{soln}H$ = enthalpy of solution. Here, the temperature dependence is:

$$\frac{-d\ln k_H}{d(1/T)} = \frac{\Delta_{soln}H}{R} \tag{5}$$

4   Unit conversions

Detailed information about the conversion between different units and definitions of Henry's law constants is given by *Sander* [1999]. Here is a short summary:

The commonly used unit for k_H is [M/atm] = $[\frac{mol_{aq}/dm_{aq}^3}{atm}]$. The official SI unit is $[\frac{mol_{aq}/m_{aq}^3}{Pa}]$. The conversion is:

$$\frac{k_H}{[M/atm]} = 101.325 \times \frac{k_H}{[(mol_{aq}/m_{aq}^3)/Pa]} \tag{6}$$

The relation between k_H and k_H^{cc} is:

$$\frac{T}{[K]} \times \frac{k_H}{[M/atm]} = 12.2 \times k_H^{cc} \tag{7}$$

At $T = 298.15$ K this leads to:

$$\frac{k_H}{[\text{M/atm}]} = 0.0409 \times k_H^{cc} \tag{8}$$

The commonly used unit for $k_{H,\text{inv}}^{px}$ is [atm]. The product of k_H and $k_{H,\text{inv}}^{px}$ is constant:

$$\frac{k_H}{[\text{M/atm}]} \times \frac{k_{H,\text{inv}}^{px}}{[\text{atm}]} = 55.3 \tag{9}$$

5   How to use the Tables

Inorganic substances are sorted according to the elements they contain. The order chosen is: O, H, N, F, Cl, Br, I, S, rare gases, others.

Organic substances (i.e. everything with carbon, including CO and CO_2) are sorted somewhat arbitrarily by increasing chain length and complexity. Hetero atoms (N, F, Cl, Br, I, and S) are sorted in the same way as for inorganic compounds.

The column labeled 'substance' gives the systematic name, the chemical formula, trivial names (if any), and in several cases the CAS registry number (in square brackets).

The column labeled '$k_H^{\ominus}$' contains the Henry's law constants as defined in equation (1), rounded to two significant digits and given in the unit [M/atm].

The column labeled '$-d\ln k_H/d(1/T)$' contains the temperature dependence of the Henry's law constants as defined in equations (4) and (5), rounded to two significant digits and given in the unit [K].

For each table entry the column labeled 'type' denotes how the Henry's law constant was obtained in the given reference. Literature reviews are usually most reliable, followed by original publications of experimental determinations of k_H. Other data has to be treated more carefully. The types listed here are roughly ordered by decreasing reliability:

'L'	The cited paper is a literature review.
'M'	Original publication of a measured value (e.g. head-space or bubble column technique as explained by *Betterton* [1992]).
'V'	Vapor pressure of the pure substance is used to determine the Henry's law constant (c/p for a saturated solution).
'R'	The cited paper presents a recalculation of previously published material (e.g. extrapolation to a different temperature or concentration range).
'T'	Thermodynamical calculation ($\Delta_{\text{soln}}G = -RT\ln k_H$, see *Sander* [1999] for details).
'C'	The paper that is cited here refers to another reference which I could not obtain (e.g. personal communication, Ph.D. theses, internal papers etc.).
'X'	I haven't seen the paper that I cite here. I found it referenced by another paper or I know about it through others.
'?'	The cited paper doesn't clearly state how the value was obtained.
'E'	The value is estimated. Estimates are only listed if no reliable measurements are available for that compound.

In some cases there might be good agreement between different authors. However, if the original work they refer to is not known one has to be careful when evaluating the reliability. It is possible that they were recalculating data from the same source. The similarity in that case would not be due to independent investigations.

6   Further Sources of Information

Further important references:

- monoaromatic hydrocarbons, chlorobenzenes, and PCBs: *Mackay et al.* [1992a]

- polynuclear aromatic hydrocarbons, polychlorinated dioxins, and dibenzofuranes: *Mackay et al.* [1992b]

- volatile organic chemicals: *Mackay et al.* [1993]

- oxygen, nitrogen, and sulfur containing compounds: *Mackay et al.* [1995]

- pestizides, PCB's, etc.: *Westcott et al.* [1981]; *Burkhard et al.* [1985]; *Hassett and Milicic* [1985]; *Yin and Hassett* [1986]; *Murphy et al.* [1987]; *Shiu et al.* [1988]; *Rice et al.* [1997]; *Fendinger and Glotfelty* [1988]; *Fendinger et al.* [1989]; *De Maagd et al.* [1998]; *Duce et al.* [1991]

- additional references that are not (yet) included: *Lide and Frederikse* [1995]; *Shiu et al.* [1994]; *Watts and Brimblecombe* [1987]; *Wright et al.* [1992a]; *Tse et al.* [1992]; *Kolb et al.* [1992]; *Ettre et al.* [1993]; *Gan and Yates* [1996]; *Peng and Wan* [1997]; *Roberts and Dändliker* [1983]; *Economou et al.* [1997]; *Wong and Wang* [1997]; *Suleimenov and Krupp* [1994]; *Heron et al.* [1998]; *Becker et al.* [1998]; *Leuenberger et al.* [1985]

- predictive methods for Henrys law coefficients (QSPRs): *Russell et al.* [1992]; *Nirmalakhandan et al.* [1997]; *Brennan et al.* [1998]

On the Internet:

- The NIST Chemistry WebBook at http://webbook.nist.gov/chemistry

- The Pesticide Properties Database (PPD) at http://www.arsusda.gov/rsml/ppdb2.html

| substance	$\dfrac{k_H^{\ominus}}{[M/atm]}$	$\dfrac{\frac{-d\ln k_H}{d(1/T)}}{[K]}$	reference	type	note
3-methyl butanoic acid $(CH_3)_2CHCH_2COOH$	1.2×10^3		Khan et al. [1995]	M	
2,2-dimethyl propanoic acid $(CH_3)_3CCOOH$	3.5×10^2		Khan et al. [1995]	M	
hexanoic acid $C_5H_{11}COOH$ [142-62-1]	1.4×10^3 1.2×10^3	6304 5900	Khan et al. [1995] Staudinger and Roberts [1996]	M ?	 70
propenoic acid $C_3H_4O_2$ (acrylic acid) [79-10-7]	2.4×10^3		Yaws and Yang [1992]	?	39
2-Methyl-2-propenoic acid $C_4H_6O_2$ (methacrylic acid) [79-41-4]	2.6×10^3		Khan et al. [1992]	M	
benzoic acid C_6H_5COOH	2.4×10^4 1.4×10^4	 6500	Yaws and Yang [1992] USEPA [1982]	? X	39 3
ethanedioic acid HOOCCOOH (oxalic acid)	7.0×10^6 5.0×10^8		Gaffney and Senum [1984] Saxena and Hildemann [1996]	X E	48 51
propanedioic acid $HOOCCH_2COOH$ (malonic acid)	4.0×10^8		Saxena and Hildemann [1996]	E	51
butanedioic acid $HOOC(CH_2)_2COOH$ (succinic acid)	3.0×10^8		Saxena and Hildemann [1996]	E	51
pentanedioic acid $HOOC(CH_2)_3COOH$ (glutaric acid)	2.0×10^8		Saxena and Hildemann [1996]	E	51
hexanedioic acid $HOOC(CH_2)_4COOH$ (adipic acid)	2.0×10^8 1.8×10^7	 11000	Saxena and Hildemann [1996] USEPA [1982]	E X	51 3
cis-butenedioic acid $HOOC(CH)_2COOH$ (maleic acid)	1.0×10^9		Saxena and Hildemann [1996]	E	51
ethanoic peroxyacid CH_3COOOH (peroxyacetic acid)	6.7×10^2 8.4×10^2	5900 5300	Lind and Kok [1994] O'Sullivan et al. [1996]	M M	9

9   Notes

1) The value is taken from the compilation of solubilities by W. Asman (unpublished).

2) Only the tabulated data between $T = 273$ K and $T = 303$ K from *Dean* [1992] was used to derive k_H and $-\Delta_{soln} H/R$. Above $T = 303$ K the tabulated data could not be parameterized by equation (4) very well. The partial pressure of water vapor (needed to convert some Henry's law constants) was calculated using the formula given by *Sander et al.* [1994]. The quantities A and α from *Dean* [1992] were assumed to be identical.

3) Value given here as quoted by *Staudinger and Roberts* [1996].

4) *Hoffmann and Jacob* [1984] refer to several references in their list of Henry's law constants but they don't assign them to specific species.

5) Calculated from correlation between the polarizabilities and solubilities of stable gases. The temperature dependence is an estimate of the upper limit.

6) *Jacob* [1986] assumed the temperature dependence to be the same as for water.

7) *Schwartz* [1984] gives an upper limit of $k_H = 6.8 \times 10^3$ M/atm. In the abstract a range of 1×10^3 M/atm $< k_H < 3 \times 10^3$ M/atm is given. The mean value of this range (2×10^3 M/atm) has been used by *Lelieveld and Crutzen* [1991], *Pandis and Seinfeld* [1989], and *Jacob* [1986].

8) Value at $T = 293$ K.

9) This value is a correction of the solubility published by *Lind and Kok* [1986].

10) This value was measured at low pH. It is superseded by a later publication of the same group [*Lind and Kok*, 1994].

11) Value given here as quoted by *Betterton* [1992].

12) *Bone et al.* [1983] gives *Carter et al.* [1968] as the source for the data. However, no data was found in that reference.

13) Several references are given in the list of Henry's law constants but not assigned to specific species.

14) The parametrization given by *Lide and Frederikse* [1995] (parameters A, B, C) doesn't fit the data in the same paper for this substance. Therefore the parametriztaion of the solubility data (X_1) was recalculated.

15) Value at $T = 295$ K.

16) Value obtained by estimating the diffusion coefficient for NO_3 to be $D = 1.0 \times 10^{-5}$ cm^2/s.

17) The value given by *Seinfeld and Pandis* [1998] is wrong.

18) The assumption of irreversible hydrolysis is equivalent to an infinite effective Henry's law constant.

19) This value was extrapolated from data at $T = 230$ K and $T = 273$ K.

20) For strong acids, the solubility is often expressed as $k_H = ([H^+] + [A^-])/p(HA)$. To obtain the physical solubility of HA, the value has to be divided by the acidity constant K_A.

21) *Brimblecombe and Clegg* [1989] corrects erroneous data from *Brimblecombe and Clegg* [1988].

22) *Lelieveld and Crutzen* [1991] assume the temperature dependence to be the same as for $a(H^+)a(NO_3^-)/p(HNO_3)$ in *Schwartz and White* [1981].

23) *Möller and Mauersberger* [1992] assumed the solubility to be comparable to HNO_3.

24) This value was extrapolated from data at $T = 215$ K and $T = 263$ K.

25) fitting parameter used in numerical modeling.

26) *Kruis and May* [1962] claim that Cl_2 does not obey Henry's law. Looking at their interpolation formula, however, it seems that this is only because they did not consider the equilibrium $Cl_2 + H_2O \rightleftharpoons HOCl + HCl$.

27) *Chameides and Stelson* [1992] refer to *Jacob* [1986] and *Chameides* [1984] but this value cannot be found there.

28) Data from Table 1 in preprint of the paper. *J. Geophys. Res.* forgot to print the tables.

29) *Fickert* [1998] extracted a value for HOBr from wetted-wall flow tube experiments. However, it was later discovered that under the experimental conditions no evaluation of k_H is possible (J. Crowley, pers. comm., 1999).

30) As quoted by *Kruis and May* [1962].

31) *Dubik et al.* [1987] measured the solubility in concentrated salt solutions (natural brines).

32) This work, using data from *Wagman et al.* [1982] and the aqueous-phase equilibrium $Cl_2 + Br_2 \rightleftharpoons 2\,BrCl$ from *Wang et al.* [1994].

33) Calculated by R. Vogt (pers. comm., 1996), using data from *Wagman et al.* [1982] and the aqueous-phase equilibrium $BrCl + Br^- \rightleftharpoons Br_2Cl^-$ from *Wang et al.* [1994].

34) Value at $T = 290$ K.

35) *Thompson and Zafiriou* [1983] quote a paper as the source that gives only the solubility but not the Henry's law constant.

36) *Gmitro and Vermeulen* [1964] give partial pressures of H_2SO_4 over a concentrated solution (e.g. 10^{-7} mmHg for 70 weight-percent at 298 K). Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for k_H.

37) Interpolation of the original data at $T < 300$ K. According to *Morrison and Johnstone* [1954] the solubility increases at higher temperatures.

38) Value at $T = 288$ K.

39) *Yaws and Yang* [1992] give several references for the Henry's law constants but don't assign them to specific species.

40) *Hansen et al.* [1995] found that the solubility of 2-methylhexane increses with temperature.

41) Value at $T = 294$ K.

42) Value given here as quoted by *Wasik and Tsang* [1970].

43) *Karl and Lindinger* [1997] also measured solubilities in salt solutions.

44) The value given by *Wilhelm et al.* [1977] is wrong.

45) Value given here as cited in *Dewulf et al.* [1995].

46) This paper supersedes earlier work with more concentrated solutions [*Butler et al.*, 1933].

47) Value given here as quoted by *Hine and Weimar* [1965].

48) Value given here as quoted by *Gaffney et al.* [1987].

49) Value at $T = 303$ K.

50) *Koga* [1995] found that *tert*-butanol does not obey Henry's law at c > 3.8 mM.

51) Value obtained by *Saxena and Hildemann* [1996] using the group contribution method.

52) Value at $T = 307$ K.

53) Value given here as quoted by *Hine and Mookerjee* [1975].

54) It is assumed here that the thermodynamic data in *Parsons et al.* [1971] refers to the units $[mol\,dm^{-3}]$ and [atm] as standard states.

55) Value given here as quoted by *Lüttke and Levsen* [1997].

56) It is assumed here that the thermodynamic data in *Parsons et al.* [1972] refers to the units $[mol\,dm^{-3}]$ and [atm] as standard states.

57) *Saxena and Hildemann* [1996] say that this value is unreliable.

58) Value given here as quoted by *Mackay et al.* [1995].

59) *Jacob* [1986] assumes $k_H(CH_3OO) = k_H(CH_3OOH) \times k_H(HO_2)/k_H(H_2O_2)$.

60) *Lelieveld and Crutzen* [1991] assume $k_H(CH_3OO) = k_H(HO_2)$.

61) *Ledbury and Blair* [1925] (and also *Blair and Ledbury* [1925]) measured the solubility of HCHO at very high concentrations around 5 to 15 M. Their value of k_H increases with HCHO concentration. *Lelieveld and Crutzen* [1991], *Hough* [1991], and *Pandis and Seinfeld* [1989] all use these solubility data but do not specify how they extrapolated to lower concentrations. Since the concentration range is far away from typical values in atmospheric chemistry the data is not reproduced here.

62) *Dong and Dasgupta* [1986] found that the Henry's law constant for HCHO is not a true constant but increases with increasing concentration. They recommend the expression

$$[HCHO] = 10^{(4538/T - 11.34)} \times p(HCHO)^{(252.2/T + 0.2088)}$$

A R E S
CORPORATION

CALCULATION
SHEET

PROJECT NO.: ACID DISSOLUTION   CALC NO.: 0193101.07-CH-001   REVISION NO.: 1   SHEET NO.: 1 OF 7

SUBJECT: MOLAR FRACTION OF OXALIC ACID IN VAPOR PHASE FOR TANK C-106 ACID DISSOLUTION PROJECT

PREPARED BY: M. FELDMANN   DATE: 7/17/03   REVIEWED BY: T.SALZANO   DATE: 7/22/03

Attachment B

Temperature Data for Tank C-106

Temperature Data for Tank C-106 from TWINS Database

Tank Name	Measurement Date	Reading	Units	Quality Indicator	Sensor Type	Location	Thermocouple Number
C106	6/10/03 4:01	79.88	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	4
C106	6/10/03 4:01	80.06	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	5
C106	6/10/03 4:01	80.6	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	6
C106	6/10/03 4:01	82.4	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	1
C106	6/10/03 4:01	79.52	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	2
C106	6/11/03 4:01	82.76	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	1
C106	6/11/03 4:01	80.06	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	2
C106	6/11/03 4:01	80.06	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	4
C106	6/11/03 4:01	80.42	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	5
C106	6/11/03 4:01	80.6	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	6
C106	6/12/03 4:02	81.68	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	6
C106	6/12/03 4:02	83.84	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	1
C106	6/12/03 4:02	81.14	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	2
C106	6/12/03 4:02	81.14	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	4
C106	6/12/03 4:02	81.5	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	5
C106	6/13/03 4:02	76.82	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	1
C106	6/13/03 4:02	76.28	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	2
C106	6/13/03 4:02	77.18	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	4
C106	6/13/03 4:02	77.36	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	5
C106	6/13/03 4:02	78.08	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	6
C106	6/14/03 4:02	78.44	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	1
C106	6/14/03 4:02	77.9	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	2
C106	6/14/03 4:02	78.26	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	4
C106	6/14/03 4:02	78.8	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	5
C106	6/14/03 4:02	78.8	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	6
C106	6/15/03 4:02	80.06	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	1
C106	6/15/03 4:02	78.8	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	2
C106	6/15/03 4:02	79.16	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	4
C106	6/15/03 4:02	79.52	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	5
C106	6/15/03 4:02	79.7	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	6
C106	6/16/03 4:02	81.14	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	1
C106	6/16/03 4:02	79.7	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	2
C106	6/16/03 4:02	79.88	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	4
C106	6/16/03 4:02	80.24	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	5
C106	6/16/03 4:02	80.42	Fahrenheit	G	Temperature (E - Type)	241-C-106-RISER-8	6

Average Temperature   79.8   Fahrenheit
26.5   Celsius

Reference:

Tank Waste Information Network System (TWINS), Queried 06/24/03,
[Tank 241-C-106, Temperature Data from 6/10/03 to 6/16/03, Fahrenheit], http://twins.pnl.gov:8001/twins.htm.